

# Deriving local order parameters from tensor network representations

Huan-Qiang Zhou<sup>1</sup>

<sup>1</sup>*Centre for Modern Physics and Department of Physics,  
Chongqing University, Chongqing 400044, The People's Republic of China*  
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A large class of quantum phase transitions for quantum lattice systems are characterized by local order parameters. It is shown that local order parameters may be systematically constructed from tensor network representations of quantum many-body ground state wave functions by investigating the reduced density matrices for local areas on an infinite-size lattice. Depending on whether or not the system symmetries are spontaneously broken, and whether or not the ground state fidelity per lattice site is continuous, there are four categories of quantum phase transitions for systems with local order parameters. Quantum phase transitions characterized by nonlocal order parameters are discussed, aiming at better understanding quantum systems with topological order.

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Quantum phase transitions (QPTs) [1] are driven by quantum fluctuations due to the uncertainty principle, and occur at zero temperature when some control parameter varies. In the last decades, much attention has been paid to QPTs in strongly correlated electronic systems, since some of the most exciting discoveries in condensed matter physics, such as various magnetic orderings, the integer and fractional quantum Hall effects, and the high- $T_c$  superconductors, are often attributed to quantum critical phenomena. In the conventional Landau-Ginzburg-Wilson paradigm, the key notions are symmetry-breaking orders and local order parameters, with symmetry-broken phases characterized by the non-zero values of local order parameters. A new paradigm emerges for systems with topological order [2], where no local order parameter exists to characterize exotic orders.

In spite of their decisive role in characterizing QPTs, no scheme, which is applicable (at least in principle) to quantum systems undergoing QPTs, is available to systematically construct order parameters (either local or nonlocal). The only exception, to the best of our knowledge, is the work by Furukawa, Misguich and Oshikawa [3], who attempted to systematically derive order parameters from comparing the reduced density matrices of the *degenerate* ground states for various subareas of the system defined on a *finite-size* lattice. In their approach, the low-lying energy spectrum and eigenvectors of a finite-size system with a given discrete symmetry are known (analytically or numerically), where a finite number of ground states are assumed to be nearly degenerate, with their quantum numbers indicating what symmetries are broken in the thermodynamic limit. Therefore, the approach, as it stands, only works for systems with a finite number of (nearly) degenerate ground states.

The difficulties of determining order parameters for a QPT in a given quantum system lie in the facts that (i) usually it is a formidable task to compute ground state wave functions and (ii) the ground state phase diagram is often lacking. However, significant advances have

been made in both the classical simulation of quantum lattice systems and the determination of ground state phase diagrams: first, a *tensor network* (TN) representation of quantum many-body wave functions provides an efficient way to classically simulate quantum many-body systems [4, 5, 6, 7, 8, 9, 10, 11]; second, two novel approaches to study QPTs have been proposed from a quantum information perspective, namely *entanglement* [12, 13, 14, 15, 16, 17, 18] and *fidelity* [19, 20, 21, 22, 23]. In Ref. [22], a viable scheme to determine the ground state phase diagram of a quantum lattice system without prior knowledge of order parameters was proposed. This was achieved by studying the singularities in the ground state fidelity per lattice site [20], combining with a practical way to compute the fidelity per lattice site for infinite-size lattice systems using the TN algorithms for translationally invariant systems [8, 9].

In this paper, we develop a practical scheme to systematically determine local order parameters for quantum many-body systems on infinite-size lattices from tensor network representations of the ground state wave functions by investigating the reduced density matrices for local areas. It yields that there are four categories of QPTs characterized by local order parameters, depending on whether or not the ground state fidelity per lattice site is continuous, and whether or not the system symmetries are spontaneously broken. If no local order parameters exist, then the system is described by a non-local order parameter. The latter is relevant to QPTs in quantum systems with topological order.

*Local and nonlocal order parameters.* Consider a translationally invariant infinite-size quantum lattice system  $S$  in  $D$  spatial dimensions described by a Hamiltonian  $H(\lambda)$  with a global symmetry group  $G$ , where  $\lambda$  is a control parameter [24]. Suppose the system undergoes a QPT at a transition point  $\lambda = \lambda_c$ . Then any two different ground states  $|\psi(\lambda_1)\rangle$  and  $|\psi(\lambda_2)\rangle$  corresponding to two different values  $\lambda_1$  and  $\lambda_2$  of the control parameter  $\lambda$  are orthogonal to each other, i.e.,  $\langle\psi(\lambda_2)|\psi(\lambda_1)\rangle = 0$ .

Therefore, the ground states  $|\psi(\lambda)\rangle$  for different values of the control parameter  $\lambda$  are reliably distinguishable via quantum measurements [25]. This leads to the existence of *local* physical observables, which enable to distinguish the states by means of local measurements, if sufficient copies of the system are *simultaneously* prepared [26] for *different* values of the control parameter. However, a more pertinent question is to ask if there is any local physical observable  $O$  (Hermitian and traceless) defined in a local area  $\Omega$  on the lattice that may tell us in which phase a given state  $|\psi(\lambda)\rangle$  is:  $\langle O \rangle \neq 0$  in one phase and  $\langle O \rangle = 0$  in the other phase, if copies of the system for one *single* value of the control parameter are prepared [27]. If the answer to the question is affirmative, then we may *define* the local physical observable as a *local order parameter* [28]. Depending on whether or not the fidelity per lattice site is continuous [29], and whether or not the symmetries are spontaneously broken, we have four different categories of QPTs with local order parameters: (1) discontinuous, symmetries not broken; (2) discontinuous, symmetries broken; (3) continuous, symmetries not broken; and (4) continuous, symmetries broken. If no local order parameter exists, then one may further seek a nonlocal physical observable  $O_n$  defined on a nonlocal area on the infinite-size lattice to judge in which phase a given state  $|\psi(\lambda)\rangle$  is, with only copies of the system prepared for one *single* value of the control parameter. Such a nonlocal physical observable  $O_n$  is a *nonlocal order parameter*. This accommodates systems with exotic topological order [30], which may even coexist with local symmetry-breaking orders.

*Reduced density matrices for local areas on an infinite lattice.* Now we are in a position to clarify what consequences one may draw from the existence of a local order parameter  $\langle O \rangle$  on a local area  $\Omega$ . Here we emphasize that, due to translational invariance, what really matters is only the size and shape of the area  $\Omega$ , rather than its relative position in the entire lattice. For our purpose, we partition the whole system into two parts—the local area  $\Omega$  and its complement to the entire lattice  $\bar{\Omega}$ . As such, the local area  $\Omega$  is described by the reduced density matrix  $\rho_\Omega(\lambda)$  corresponding to a given ground state  $|\psi(\lambda)\rangle$ . Generically, the reduced density matrix  $\rho_\Omega(\lambda)$  exhibits nontrivial form due to the distinguishability by local measurements [26], except for the constraints imposed by the global symmetries (in the symmetric phase). An important fact is that the reduced density matrix  $\rho_\Omega(\lambda)$  possesses different *structures* in two phases as far as the nonzero entries are concerned:  $\rho_\Omega(\lambda) = \rho_{\Omega 0}(\lambda)$  in one phase and  $\rho_\Omega(\lambda) = \rho_{\Omega 0}(\lambda) + \langle O \rangle O / (\text{Tr} O^2)$  in the other phase, as follows from the presence of the local order parameter  $\langle O \rangle$ . Two cases should be distinguished: (i) if  $O$  is not invariant under the symmetry transformation, then the symmetry is spontaneously broken; (ii) if  $O$  is invariant under the symmetry transformation, then no symmetry is broken.

We stress that local order parameters are not unique. Indeed, suppose a local order parameter  $\langle O \rangle$  exists for a local area  $\Omega$ , then there exists another local order parameter  $\langle \tilde{O} \rangle$  for a larger area  $\tilde{\Omega} \supset \Omega$ , since all information encoded in the reduced density matrix  $\rho_\Omega(\lambda)$  should be encoded in the reduced density matrix  $\rho_{\tilde{\Omega}}(\lambda)$ , due to the fact that  $\rho_\Omega(\lambda)$  is obtained from  $\rho_{\tilde{\Omega}}(\lambda)$  by tracing out extra degrees of freedom in the complement set  $\tilde{\Omega}/\Omega$ . This implies that there is an *optimal* local order parameter that corresponds to the smallest local area for the system considered [31].

On the other hand, if the reduced density matrices for all possible local areas share the *same* nonzero entries structure in two phases, then a *nonlocal* order parameter is necessary to characterize the QPT. That is, an area with nontrivial topology should be chosen to see if the corresponding reduced density matrices exhibit different structures in different phases [32].

*Computation of the reduced density matrices from tensor network representations.* Now we show that it is feasible to compute the reduced density matrices for various local areas on infinite-size lattices. In this regard, we rely heavily on the fact that the TN representation of quantum many-body wave functions provides a powerful means to efficiently simulate infinite-size quantum lattice systems in one [8] and two and higher [9] spatial dimensions. In one spatial dimension, the NT representation is the matrix product states (MPS) [4], and, in two and higher spatial dimensions, the NT representation is the projected entangled-pair states (PEPS) [7]. In both cases, the TN algorithms for infinite-size lattices offer an efficient way to compute the reduced density matrices for various local areas, if quantum lattice systems are in gapful phases.

If quantum lattice systems are in gapless phases, then a more sophisticated representation, i.e., the multi-scale entanglement renormalization ansatz (MERA) [10, 11] is needed for quantum many-body states. A MERA also provides an efficient representation of quantum ground states on an infinite-size lattice. Thanks to the fact that the width of the causal cone is bounded, a MERA offers an efficient way to compute the reduced density matrices for various local areas. In Ref. [10], it is described explicitly how to compute the one-site and two-site reduced density matrices from a MERA.

*A practical scheme to derive local order parameters from tensor network representations.* For a quantum lattice system with a symmetry group  $G$ , one may systematically derive local order parameters from the TN representations of quantum many body ground state wave functions. It consists of two steps: (1) determine the ground state phase diagram by computing the ground state fidelity per lattice site in terms of the infinite TN algorithms [22]; (2) derive local order parameters from a representative ground state wave functions by investigating the reduced density matrices for local areas on an

infinite-size lattice.

To be self-contained, let us briefly recall the definition of the ground state fidelity per lattice site  $d(\lambda_1, \lambda_2)$ . For any two ground states  $|\psi(\lambda_1)\rangle$  and  $|\psi(\lambda_2)\rangle$ , the fidelity  $F(\lambda_1, \lambda_2)$  asymptotically scales as  $F(\lambda_1, \lambda_2) \sim d(\lambda_1, \lambda_2)^N$ , with  $N$  the total number of sites in the lattice. Here  $d(\lambda_1, \lambda_2)$  is the fidelity per lattice site [20, 22], which is well defined in the thermodynamic limit:

$$d(\lambda_1, \lambda_2) = \lim_{N \rightarrow \infty} F^{\frac{1}{N}}(\lambda_1, \lambda_2). \quad (1)$$

It satisfies the properties inherited from the fidelity  $F(\lambda_1, \lambda_2)$ : (i) normalization  $d(\lambda_1, \lambda_1) = 1$ ; (ii) symmetry  $d(\lambda_1, \lambda_2) = d(\lambda_2, \lambda_1)$ ; and (iii) range  $0 \leq d(\lambda_1, \lambda_2) \leq 1$ . In fact, the ground state fidelity  $F(\lambda_1, \lambda_2)$  may be mapped onto the partition function of a  $D$ -dimensional classical statistical vertex lattice model with the same geometry [22]. Thus, the fidelity per lattice site  $d(\lambda_1, \lambda_2)$  is nothing but the partition function per site in the classical statistical vertex lattice model [33]. This justifies why QPTs may be detected as singularities in  $\ln d(\lambda_1, \lambda_2)$  as a function of  $\lambda_1$  and  $\lambda_2$ .

Once the ground state phase diagram is determined, one may choose a representative ground state from each phase and investigate the reduced density matrix for a local area  $\Omega$  on an infinite-size lattice. If the nonzero entries structures of the reduced density matrices for a given local area  $\Omega$  are different for different phases, then one may read off a local order parameter: (i) if the reduced density matrices are invariant under the symmetry group  $G$ , then no symmetry is spontaneously broken (and the ground state is non-degenerate); (ii) if one of the reduced density matrices is not invariant under the symmetry group  $G$ , then the symmetry is spontaneously broken (and degenerate ground states arise). If the nonzero entries structure of the reduced density matrices for all possible local areas  $\Omega$  is the same for different phases, then there is no local order parameter [34], and vice versa. For systems with topological order, this is consistent with the fact that different states in the ground state subspace share the same bulk tensors in the TN representations, with the only difference at the top tensor [35].

*Examples.* Let us give a few examples to illustrate our general scheme. The first example is the two-dimensional quantum Ising model described by the Hamiltonian:

$$H = - \sum_{(\vec{r}, \vec{r}')} \sigma_z^{[\vec{r}]} \sigma_z^{[\vec{r}']} - \lambda \sum_{\vec{r}} \sigma_x^{[\vec{r}]} - \epsilon \sum_{\vec{r}} \sigma_z^{[\vec{r}]} \quad (2)$$

Here  $\sigma_x^{[\vec{r}]}$  and  $\sigma_z^{[\vec{r}]}$  are the Pauli matrices at the lattice site  $\vec{r}$ , and the control parameters  $\lambda$  and  $\epsilon$  correspond to transverse and parallel magnetic fields. Note that if  $\epsilon = 0$ , then the model enjoys the  $Z_2$  symmetry; otherwise no symmetry exists. As shown in Ref. [22], for  $\epsilon = 0$ , the fidelity per site  $d(\lambda_1, \lambda_2)$  is continuous, but it exhibits a *pinch point* singularity, indicating a continuous phase transition at  $\lambda_c \approx 3.044$  [36]. On the

other hand, the one-site reduced density matrix  $\rho_1$  displays different nonzero-entries structures in two phases:  $\rho_1^{[\vec{r}]} = 1/2 + 1/2 \langle \sigma_x^{[\vec{r}]} \rangle \sigma_x + 1/2 \langle \sigma_z^{[\vec{r}]} \rangle \sigma_z$ , with  $\langle \sigma_z^{[\vec{r}]} \rangle$  being zero for  $\lambda > \lambda_c$  and nonzero for  $\lambda < \lambda_c$ , as evaluated using the infinite TN algorithm in Ref. [9].  $\rho_1$  is non-trivial under the global  $Z_2$  symmetry transformation, so the  $Z_2$  symmetry is spontaneously broken. This implies the existence of a local order parameter:  $\langle O \rangle = \langle \sigma_z^{[\vec{r}]} \rangle$ . For nonzero  $\epsilon$ , when  $\lambda < \lambda_c$ , the fidelity per site  $d(\epsilon_1, \epsilon_2)$  is discontinuous [22], implying that a first order QPT occurs when  $\epsilon$  changes sign. The one-site reduced density matrix  $\rho_1$  displays different structures in different phases:  $\langle \sigma_z^{[\vec{r}]} \rangle$  changes sign, since the symmetry group is trivial [27].

The second example is a spin 1/2 model with three-body interactions:

$$H = \sum_i 2(g^2 - 1) \sigma_i^z \sigma_{i+1}^z - (1+g)^2 \sigma_i^x + (g-1)^2 \sigma_i^z \sigma_{i+1}^x \sigma_{i+2}^z. \quad (3)$$

It is  $Z_2$ -symmetric under the global spin reversal in the  $z$  direction. As emphasized in Ref. [20], the parameter space should be compactified by identifying  $g = +\infty$  with  $g = -\infty$ , due to the fact that  $H(+\infty) = H(-\infty)$ . Since the ground state is an MPS [37], one may extract the fidelity per site  $d$  as  $d(g, g') = \sqrt{1 + |gg'|} / \sqrt{(1 + |g|)(1 + |g'|)}$  if  $g$  and  $g'$  are in different phases, and  $d(g, g') = (1 + \sqrt{|gg'|}) / \sqrt{(1 + |g|)(1 + |g'|)}$  if  $g$  and  $g'$  are in the same phase. Thus there are two transition points:  $g = 0$  and  $\infty$ . All states for positive  $g$  flow to the product state ( $g = 1$ ) with all spins aligning in the  $x$  direction, and all states for negative  $g$  flow to the cluster state [38] ( $g = -1$ ). Since the ground state is unique, so no symmetry is spontaneously broken. Therefore, the reduced density matrices should be invariant under the  $Z_2$  symmetry group. Actually, the one-site reduced density matrix  $\rho_1$  exhibits different nonzero entries structures in different phases:  $\rho_1(i) = 1/2 + 1/2 \langle \sigma_i^x \rangle \sigma_x$ , with  $\langle \sigma_i^x \rangle = 4g/(1+g)^2$  for  $g > 0$  and  $\langle \sigma_i^x \rangle = 0$  for  $g < 0$ , thus leading to the local order parameter  $\langle \sigma_i^x \rangle$ .

The third example is the spin 1  $XXZ$  model with uniaxial single-ion anisotropy described by the Hamiltonian:

$$H = \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) + D \sum_i S_i^z{}^2, \quad (4)$$

where  $S_i^\alpha$  ( $\alpha = x, y, z$ ) are the spin 1 operators at the lattice site  $i$ , and  $J_z$  and  $D$  are the Ising-like and single-ion anisotropies, respectively. The model exhibits rich phases [39, 40, 41, 42]. For  $J_z > 0$ , three gapful phases, i.e., the large- $D$ , the Haldane, and the Néel phases occur, which have the symmetric, fully broken and partially broken  $Z_2 \times Z_2$  symmetry, respectively. It has been argued that there is a tricritical point  $(J_t, D_t) \approx (3.20, 2.90)$  [41, 42]. If  $J_z < J_t$ , then there are two critical values  $D_{c1}$  and  $D_{c2}$  when  $D$  varies from  $-\infty$  to  $\infty$ , characterizing the Ising-like transition from the Néel phase to

the Haldane phase and the Gaussian transition from the Haldane phase to the large- $D$  phase, respectively. Beyond the tricritical point where the Haldane phase disappears, the large- $D$ -Néel transition was believed to be first order, although no final proof is available [42]. This has been confirmed numerically by evaluating the fidelity per site based on the infinite TN algorithm [43]. The one-site reduced density matrix  $\rho_1$  exhibits different nonzerononzero entries structures in different phases: it is invariant under the spin reversal  $Z_2$  symmetry in the large- $D$  phase, but not in the Néel phase. This indicates that the  $Z_2$  symmetry is spontaneously broken, with a local order parameter  $\langle O \rangle = (-1)^i \langle S_i^z \rangle$ . No local order parameter exists in the Haldane phase [44].

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  - [27] Actually, this is valid for local order parameters in systems with a nontrivial symmetry group  $G$ . However, if the symmetry group  $G$  is explicitly broken, then a first-order QPT occurs, due to the presence of the term linear in  $O$ , we require that  $\langle O \rangle > 0$  in one phase and  $\langle O \rangle < 0$  in the other phase, if only copies of the system are prepared for one *single* value of the control parameter.
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  - [29] As argued in [20, 22], the discontinuity in the fidelity per lattice site corresponds to the first order QPTs.
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